N-Ethylglycine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.28 days

Global applicability domain: Outside

Local applicability domain index: 2.89e-01

Confidence level: 7.73e-01

Nearest Neighbors from the Training Set

Image not found
Tetradeca-1,13-diene
Measured: 367
Predicted: 8.69

Image not found
2-Methylhexane
Measured: 12.5
Predicted: 5.54

Image not found
1-Methyl-2-propylbenzene
Measured: 12.5
Predicted: 3.17

Image not found
Propylbenzene
Measured: 24.3
Predicted: 4.02

Image not found
2-Methylheptane
Measured: 12.5
Predicted: 3.99